



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:37 PM UTC

PDB ID : 4NBU / pdb_00004nbu
Title : Crystal structure of FabG from Bacillus sp
Authors : Pereira, J.H.; Mcandrew, R.P.; Javidpour, P.; Beller, H.R.; Adams, P.D.
Deposited on : 2013-10-23
Resolution : 1.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

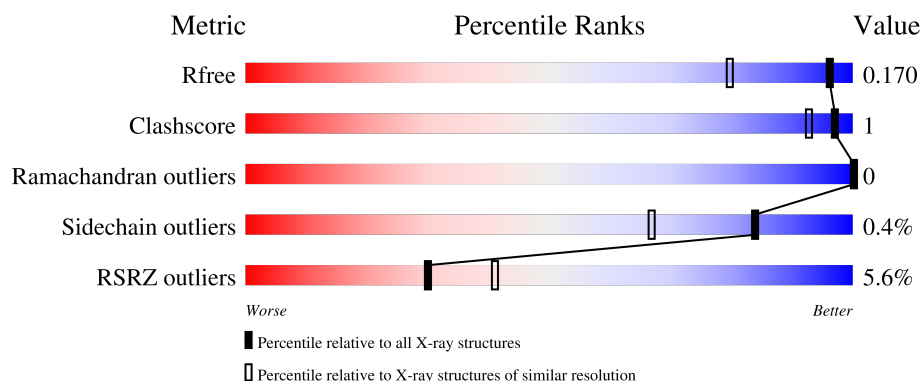
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	4% 95% ..
1	B	250	6% 94% ..
1	C	250	6% 94% ..
1	D	250	5% 94% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8527 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-oxoacyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	5	0
			1845	1164	323	347	11			
1	B	244	Total	C	N	O	S	0	4	0
			1861	1170	329	350	12			
1	C	242	Total	C	N	O	S	0	2	0
			1829	1152	321	345	11			
1	D	242	Total	C	N	O	S	0	1	0
			1824	1147	321	345	11			

There are 28 discrepancies between the modelled and reference sequences:

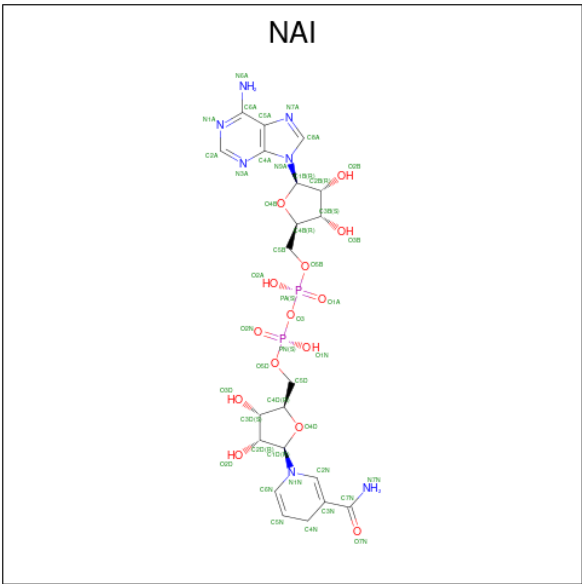
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A6CQL2
A	2	HIS	-	expression tag	UNP A6CQL2
A	3	HIS	-	expression tag	UNP A6CQL2
A	4	HIS	-	expression tag	UNP A6CQL2
A	5	HIS	-	expression tag	UNP A6CQL2
A	6	HIS	-	expression tag	UNP A6CQL2
A	7	HIS	-	expression tag	UNP A6CQL2
B	1	MET	-	expression tag	UNP A6CQL2
B	2	HIS	-	expression tag	UNP A6CQL2
B	3	HIS	-	expression tag	UNP A6CQL2
B	4	HIS	-	expression tag	UNP A6CQL2
B	5	HIS	-	expression tag	UNP A6CQL2
B	6	HIS	-	expression tag	UNP A6CQL2
B	7	HIS	-	expression tag	UNP A6CQL2
C	1	MET	-	expression tag	UNP A6CQL2
C	2	HIS	-	expression tag	UNP A6CQL2
C	3	HIS	-	expression tag	UNP A6CQL2
C	4	HIS	-	expression tag	UNP A6CQL2
C	5	HIS	-	expression tag	UNP A6CQL2
C	6	HIS	-	expression tag	UNP A6CQL2
C	7	HIS	-	expression tag	UNP A6CQL2

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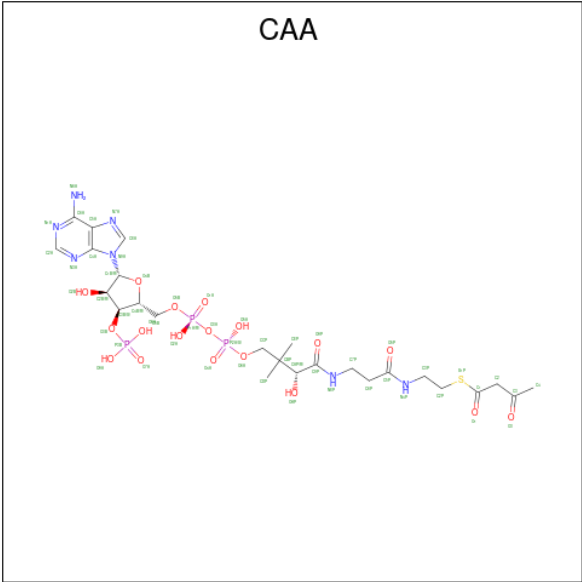
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP A6CQL2
D	2	HIS	-	expression tag	UNP A6CQL2
D	3	HIS	-	expression tag	UNP A6CQL2
D	4	HIS	-	expression tag	UNP A6CQL2
D	5	HIS	-	expression tag	UNP A6CQL2
D	6	HIS	-	expression tag	UNP A6CQL2
D	7	HIS	-	expression tag	UNP A6CQL2

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: C₂₅H₄₀N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	
			54	25	7	18	3	1	

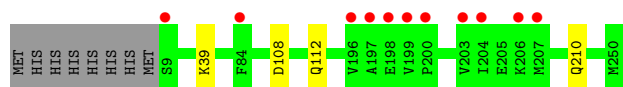
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	0
			213	213		
4	B	252	Total	O	0	0
			252	252		
4	C	230	Total	O	0	0
			230	230		
4	D	243	Total	O	0	0
			243	243		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



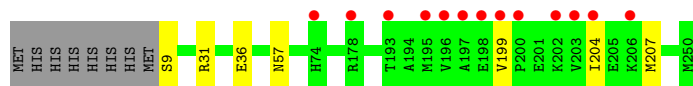
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



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- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.41Å 68.77Å 70.00Å 67.85° 88.65° 62.64°	Depositor
Resolution (Å)	23.32 – 1.34 23.32 – 1.34	Depositor EDS
% Data completeness (in resolution range)	93.7 (23.32-1.34) 88.6 (23.32-1.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1405)	Depositor
R, R_{free}	0.156 , 0.164 (Not available) , 0.170	Depositor DCC
R_{free} test set	2006 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8527	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAA, NAI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/1886	0.69	0/2547
1	B	0.40	0/1900	0.66	0/2564
1	C	0.40	0/1861	0.69	0/2513
1	D	0.40	0/1853	0.66	0/2502
All	All	0.40	0/7500	0.68	0/10126

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1845	0	1886	3	0
1	B	1861	0	1891	4	0
1	C	1829	0	1861	4	0
1	D	1824	0	1850	3	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
3	B	54	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	213	0	0	1	0
4	B	252	0	0	0	0
4	C	230	0	0	0	0
4	D	243	0	0	0	0
All	All	8527	0	7632	14	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:HA	1:D:207:MET:HE2	1.72	0.70
1:C:108:ASP:OD2	1:C:112:GLN:NE2	2.37	0.57
1:A:108:ASP:OD2	1:A:112:GLN:NE2	2.36	0.56
1:A:210:GLN:HE22	1:B:210:GLN:HE22	1.54	0.54
1:C:108:ASP:CG	1:C:112:GLN:HE21	2.20	0.49
1:C:202:LYS:O	1:C:206:LYS:HD3	2.17	0.45
1:B:196:VAL:O	1:B:199:VAL:HG22	2.18	0.43
1:A:39:LYS:NZ	4:A:478:HOH:O	2.50	0.43
1:D:31:ARG:NH1	1:D:57:ASN:OD1	2.52	0.42
1:C:196:VAL:O	1:C:199:VAL:HG22	2.21	0.41
1:B:200:PRO:O	1:B:203:VAL:HG12	2.20	0.41
1:D:9:SER:HB3	1:D:36:GLU:O	2.20	0.41
1:B:125:THR:HG23	1:B:140:ILE:HD13	2.02	0.41
3:B:302:CAA:O1	3:B:302:CAA:H31	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/250 (98%)	240 (98%)	5 (2%)	0	100	100
1	B	246/250 (98%)	239 (97%)	7 (3%)	0	100	100
1	C	242/250 (97%)	237 (98%)	5 (2%)	0	100	100
1	D	241/250 (96%)	236 (98%)	5 (2%)	0	100	100
All	All	974/1000 (97%)	952 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/198 (98%)	195 (100%)	0	100	100
1	B	196/198 (99%)	195 (100%)	1 (0%)	81	61
1	C	192/198 (97%)	191 (100%)	1 (0%)	81	61
1	D	191/198 (96%)	190 (100%)	1 (0%)	81	61
All	All	774/792 (98%)	771 (100%)	3 (0%)	84	67

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	GLU
1	C	199	VAL
1	D	199	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	152	ASN
1	A	155	GLN
1	A	210	GLN

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	93	ASN
1	B	152	ASN
1	B	155	GLN
1	C	23	ASN
1	C	93	ASN
1	C	111	GLN
1	C	210	GLN
1	D	93	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAI	D	301	-	47,48,48	1.33	7 (14%)	64,73,73	1.67	12 (18%)
3	CAA	B	302	-	53,56,56	2.20	14 (26%)	77,83,83	2.71	17 (22%)
2	NAI	B	301	-	47,48,48	1.29	4 (8%)	64,73,73	1.54	13 (20%)
2	NAI	C	301	-	47,48,48	1.33	7 (14%)	64,73,73	1.63	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	A	301	-	47,48,48	1.35	7 (14%)	64,73,73	1.60	11 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	D	301	-	-	5/29/72/72	0/5/5/5
3	CAA	B	302	-	-	17/55/71/71	0/3/3/3
2	NAI	B	301	-	-	6/29/72/72	0/5/5/5
2	NAI	C	301	-	-	6/29/72/72	0/5/5/5
2	NAI	A	301	-	-	7/29/72/72	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	CAA	C8A-N9A	-6.78	1.26	1.37
3	B	302	CAA	C9P-N8P	5.49	1.46	1.33
3	B	302	CAA	C4A-N9A	-5.41	1.26	1.37
3	B	302	CAA	C5P-N4P	4.78	1.44	1.33
3	B	302	CAA	C5A-N7A	4.20	1.46	1.39
3	B	302	CAA	C5A-C4A	4.17	1.46	1.39
2	A	301	NAI	C6A-N6A	3.69	1.43	1.34
2	D	301	NAI	C6A-N6A	3.68	1.43	1.34
3	B	302	CAA	P2A-O3A	3.65	1.63	1.59
2	C	301	NAI	C6A-N6A	3.40	1.42	1.34
2	B	301	NAI	C6A-N6A	3.38	1.42	1.34
3	B	302	CAA	O4B-C1B	3.37	1.49	1.42
2	C	301	NAI	C7N-N7N	3.21	1.42	1.33
3	B	302	CAA	C6A-N6A	3.21	1.42	1.34
2	D	301	NAI	C7N-N7N	3.11	1.42	1.33
2	A	301	NAI	C7N-N7N	3.10	1.42	1.33
2	B	301	NAI	C7N-N7N	3.03	1.42	1.33
3	B	302	CAA	OAP-CAP	-2.95	1.37	1.42
3	B	302	CAA	O4B-C4B	2.78	1.51	1.45
2	C	301	NAI	C5D-C4D	2.71	1.59	1.51
2	B	301	NAI	C5D-C4D	2.55	1.59	1.51
2	A	301	NAI	C5D-C4D	2.54	1.59	1.51
2	D	301	NAI	C5D-C4D	2.45	1.58	1.51
2	A	301	NAI	C2D-C3D	-2.31	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAI	C2D-C3D	-2.29	1.47	1.53
2	A	301	NAI	O4B-C4B	-2.27	1.39	1.45
3	B	302	CAA	C8A-N7A	2.25	1.36	1.31
3	B	302	CAA	C2B-C3B	-2.24	1.48	1.53
2	B	301	NAI	C2D-C3D	-2.22	1.47	1.53
2	D	301	NAI	C2D-C3D	-2.22	1.47	1.53
3	B	302	CAA	C3B-C4B	-2.18	1.47	1.52
2	C	301	NAI	O3D-C3D	-2.14	1.37	1.43
2	A	301	NAI	O3D-C3D	-2.14	1.37	1.43
2	C	301	NAI	O4B-C4B	-2.13	1.40	1.45
2	D	301	NAI	C5A-N7A	-2.12	1.35	1.39
2	D	301	NAI	O4B-C4B	-2.09	1.40	1.45
2	A	301	NAI	C5A-N7A	-2.07	1.35	1.39
2	D	301	NAI	O3D-C3D	-2.02	1.37	1.43
2	C	301	NAI	C5A-N7A	-2.01	1.35	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	CAA	C4A-N9A-C8A	15.40	121.91	105.74
3	B	302	CAA	N3A-C4A-N9A	7.22	139.44	127.17
3	B	302	CAA	C5A-C4A-N3A	-5.85	118.66	126.72
3	B	302	CAA	C4A-C5A-N7A	-5.67	104.10	110.58
3	B	302	CAA	N9A-C8A-N7A	-5.65	105.92	113.94
2	A	301	NAI	N3A-C2A-N1A	-5.42	120.38	128.58
2	D	301	NAI	N3A-C2A-N1A	-5.29	120.57	128.58
2	B	301	NAI	N3A-C2A-N1A	-5.03	120.97	128.58
2	C	301	NAI	N3A-C2A-N1A	-4.78	121.35	128.58
2	D	301	NAI	C5A-C4A-N3A	-4.61	120.37	126.72
2	C	301	NAI	C5A-C4A-N3A	-4.49	120.53	126.72
2	A	301	NAI	C5A-C4A-N3A	-4.43	120.62	126.72
3	B	302	CAA	N3A-C2A-N1A	-4.19	122.23	128.58
2	D	301	NAI	C5A-N7A-C8A	4.00	109.74	103.45
2	C	301	NAI	C5A-N7A-C8A	3.79	109.40	103.45
3	B	302	CAA	C2P-S1P-C1	3.75	112.92	101.84
3	B	302	CAA	C1B-N9A-C8A	-3.68	118.92	127.09
2	B	301	NAI	C5A-C4A-N3A	-3.66	121.67	126.72
3	B	302	CAA	C5A-C4A-N9A	-3.59	101.89	105.81
2	A	301	NAI	N3A-C4A-N9A	3.58	133.26	127.17
2	A	301	NAI	C5A-N7A-C8A	3.48	108.91	103.45
2	D	301	NAI	C4A-C5A-N7A	-3.41	106.69	110.58
2	C	301	NAI	N3A-C4A-N9A	3.38	132.91	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	CAA	C2A-N3A-C4A	3.34	120.00	111.83
2	A	301	NAI	C2A-N3A-C4A	3.33	119.96	111.83
2	D	301	NAI	N3A-C4A-N9A	3.33	132.83	127.17
3	B	302	CAA	C2-C1-S1P	3.31	117.83	113.63
2	D	301	NAI	C2A-N3A-C4A	3.25	119.78	111.83
2	B	301	NAI	C5A-N7A-C8A	3.24	108.54	103.45
2	D	301	NAI	N9A-C8A-N7A	-3.24	109.34	113.94
2	C	301	NAI	N9A-C8A-N7A	-3.20	109.39	113.94
3	B	302	CAA	C4A-N9A-C1B	-3.20	119.15	126.63
2	A	301	NAI	N9A-C8A-N7A	-3.15	109.46	113.94
3	B	302	CAA	C6A-C5A-N7A	3.14	138.13	132.09
2	C	301	NAI	C2A-N3A-C4A	3.13	119.47	111.83
2	C	301	NAI	C4A-C5A-N7A	-3.12	107.02	110.58
2	B	301	NAI	C2A-N3A-C4A	2.85	118.80	111.83
3	B	302	CAA	CAP-C9P-N8P	2.83	121.85	116.48
2	B	301	NAI	C1D-N1N-C2N	-2.77	116.57	121.14
2	B	301	NAI	N9A-C8A-N7A	-2.76	110.03	113.94
2	B	301	NAI	N3A-C4A-N9A	2.74	131.83	127.17
2	B	301	NAI	C4A-C5A-N7A	-2.73	107.46	110.58
2	C	301	NAI	C1D-N1N-C2N	-2.70	116.69	121.14
2	A	301	NAI	C4A-C5A-N7A	-2.61	107.60	110.58
2	C	301	NAI	C3N-C7N-N7N	2.47	122.05	117.67
3	B	302	CAA	C3B-C2B-C1B	2.40	105.17	99.89
2	A	301	NAI	O4B-C1B-N9A	2.40	112.69	108.09
2	D	301	NAI	C3N-C7N-N7N	2.37	121.88	117.67
2	A	301	NAI	C3N-C7N-N7N	2.36	121.86	117.67
2	B	301	NAI	C3N-C2N-N1N	-2.30	119.83	123.20
2	C	301	NAI	C4D-O4D-C1D	-2.28	104.43	109.47
3	B	302	CAA	O1-C1-C2	-2.27	119.62	123.40
2	B	301	NAI	C3N-C7N-N7N	2.27	121.69	117.67
2	D	301	NAI	C1D-N1N-C2N	-2.26	117.41	121.14
2	D	301	NAI	C3N-C2N-N1N	-2.23	119.92	123.20
2	D	301	NAI	O4B-C4B-C3B	2.22	109.57	105.15
2	B	301	NAI	O3-PA-O1A	-2.21	104.05	110.70
2	A	301	NAI	C4A-N9A-C8A	2.05	107.89	105.74
2	B	301	NAI	C2D-C1D-N1N	2.04	118.33	113.31
2	A	301	NAI	O4B-C4B-C3B	2.04	109.21	105.15
2	B	301	NAI	C4D-O4D-C1D	-2.03	104.98	109.47
2	D	301	NAI	C6A-C5A-N7A	2.02	135.99	132.09
3	B	302	CAA	C2B-C3B-C4B	2.01	106.76	103.24

There are no chirality outliers.

All (41) torsion outliers are listed below:

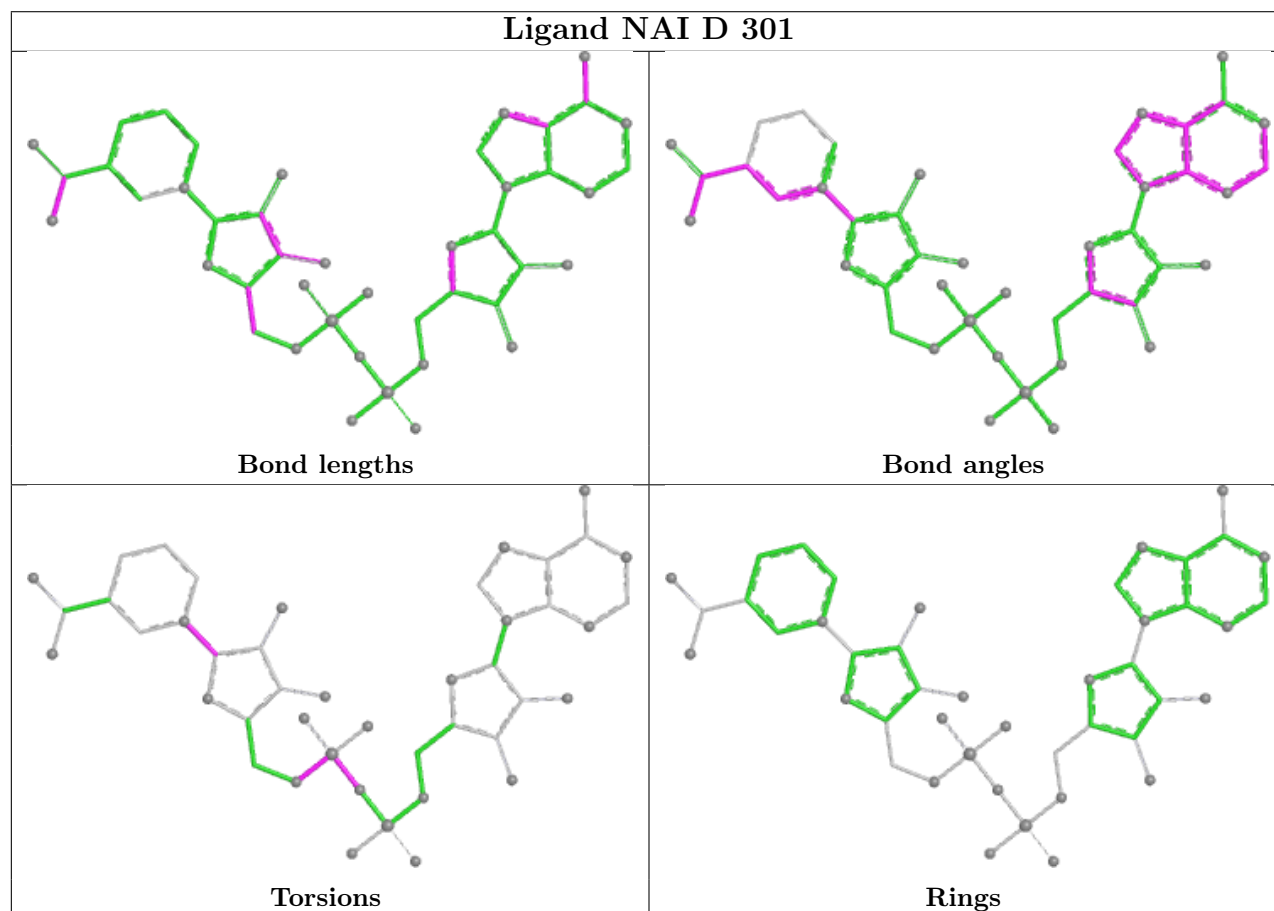
Mol	Chain	Res	Type	Atoms
2	A	301	NAI	C5D-O5D-PN-O3
2	A	301	NAI	C5D-O5D-PN-O1N
2	A	301	NAI	C5D-O5D-PN-O2N
2	B	301	NAI	C5D-O5D-PN-O3
2	B	301	NAI	C5D-O5D-PN-O1N
2	B	301	NAI	C5D-O5D-PN-O2N
2	C	301	NAI	C5D-O5D-PN-O3
2	C	301	NAI	C5D-O5D-PN-O1N
2	C	301	NAI	C5D-O5D-PN-O2N
2	D	301	NAI	C5D-O5D-PN-O3
2	D	301	NAI	C5D-O5D-PN-O1N
2	D	301	NAI	C5D-O5D-PN-O2N
3	B	302	CAA	OAP-CAP-CBP-CCP
3	B	302	CAA	C9P-CAP-CBP-CCP
3	B	302	CAA	OAP-CAP-CBP-CEP
3	B	302	CAA	C9P-CAP-CBP-CEP
3	B	302	CAA	O9P-C9P-CAP-CBP
3	B	302	CAA	N8P-C9P-CAP-CBP
3	B	302	CAA	N8P-C9P-CAP-OAP
3	B	302	CAA	S1P-C2P-C3P-N4P
3	B	302	CAA	C3P-C2P-S1P-C1
3	B	302	CAA	O1-C1-S1P-C2P
3	B	302	CAA	C2-C1-S1P-C2P
3	B	302	CAA	C1-C2-C3-O3
3	B	302	CAA	C1-C2-C3-C4
3	B	302	CAA	OAP-CAP-CBP-CDP
2	A	301	NAI	PN-O3-PA-O5B
2	B	301	NAI	PN-O3-PA-O5B
2	C	301	NAI	PN-O3-PA-O5B
3	B	302	CAA	C9P-CAP-CBP-CDP
2	B	301	NAI	O4D-C1D-N1N-C6N
2	D	301	NAI	O4D-C1D-N1N-C6N
2	A	301	NAI	O4D-C1D-N1N-C6N
2	C	301	NAI	O4D-C1D-N1N-C6N
2	D	301	NAI	PA-O3-PN-O2N
3	B	302	CAA	O5P-C5P-C6P-C7P
3	B	302	CAA	N4P-C5P-C6P-C7P
2	A	301	NAI	PA-O3-PN-O1N
2	A	301	NAI	C2N-C3N-C7N-O7N
2	B	301	NAI	PA-O3-PN-O1N
2	C	301	NAI	PA-O3-PN-O1N

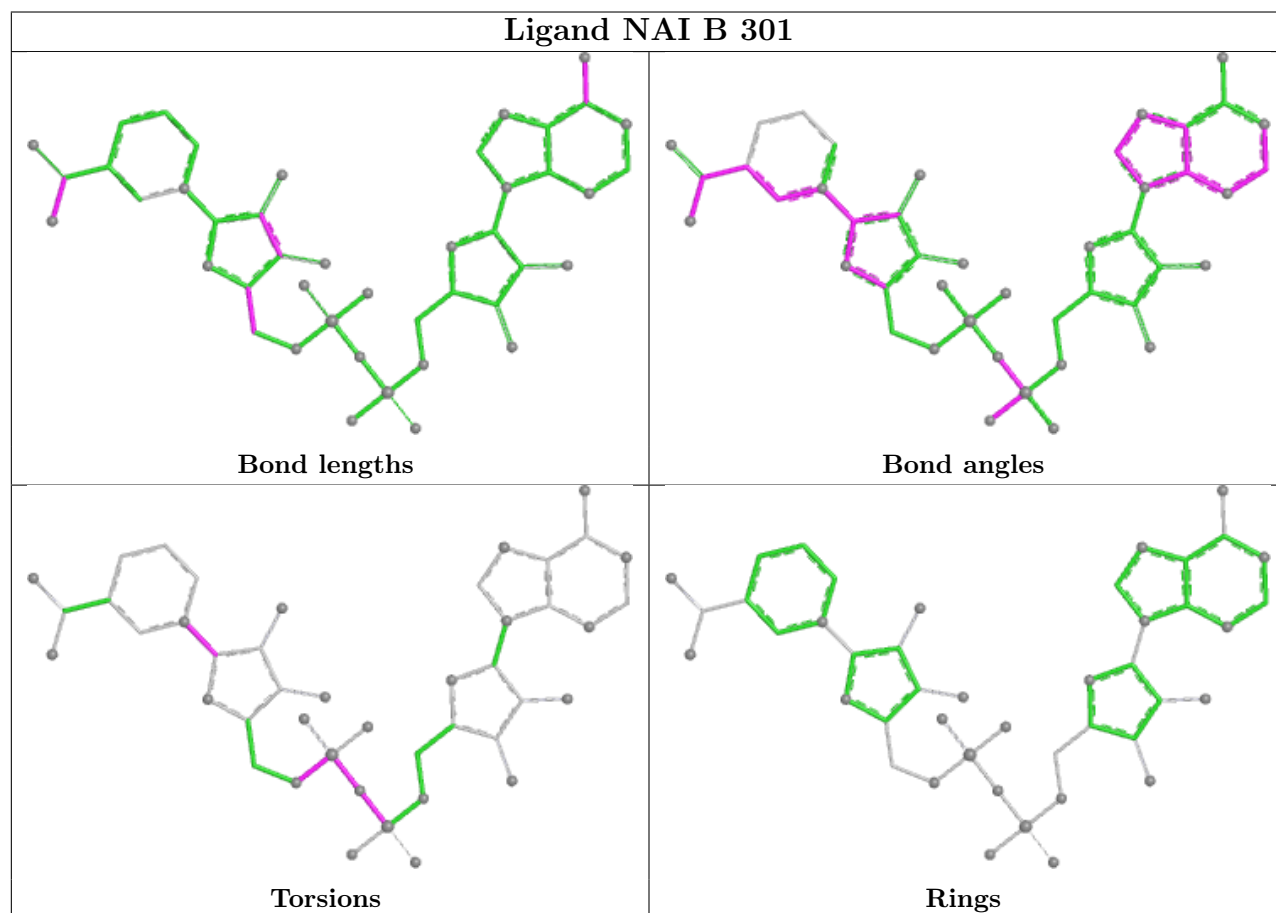
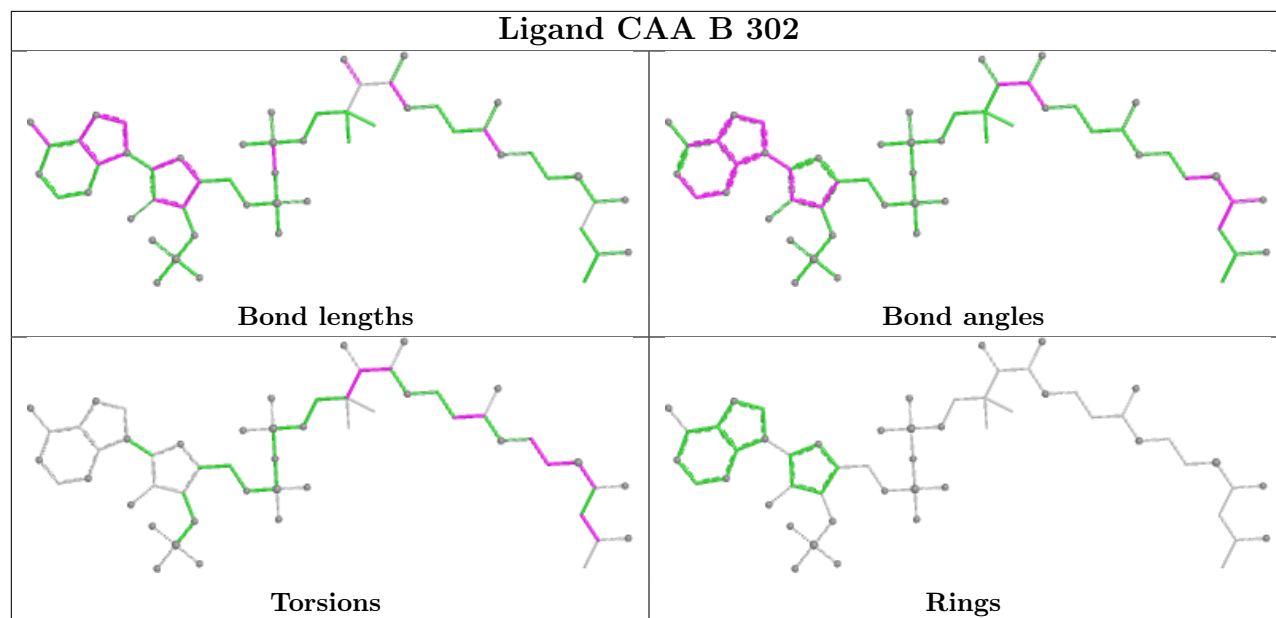
There are no ring outliers.

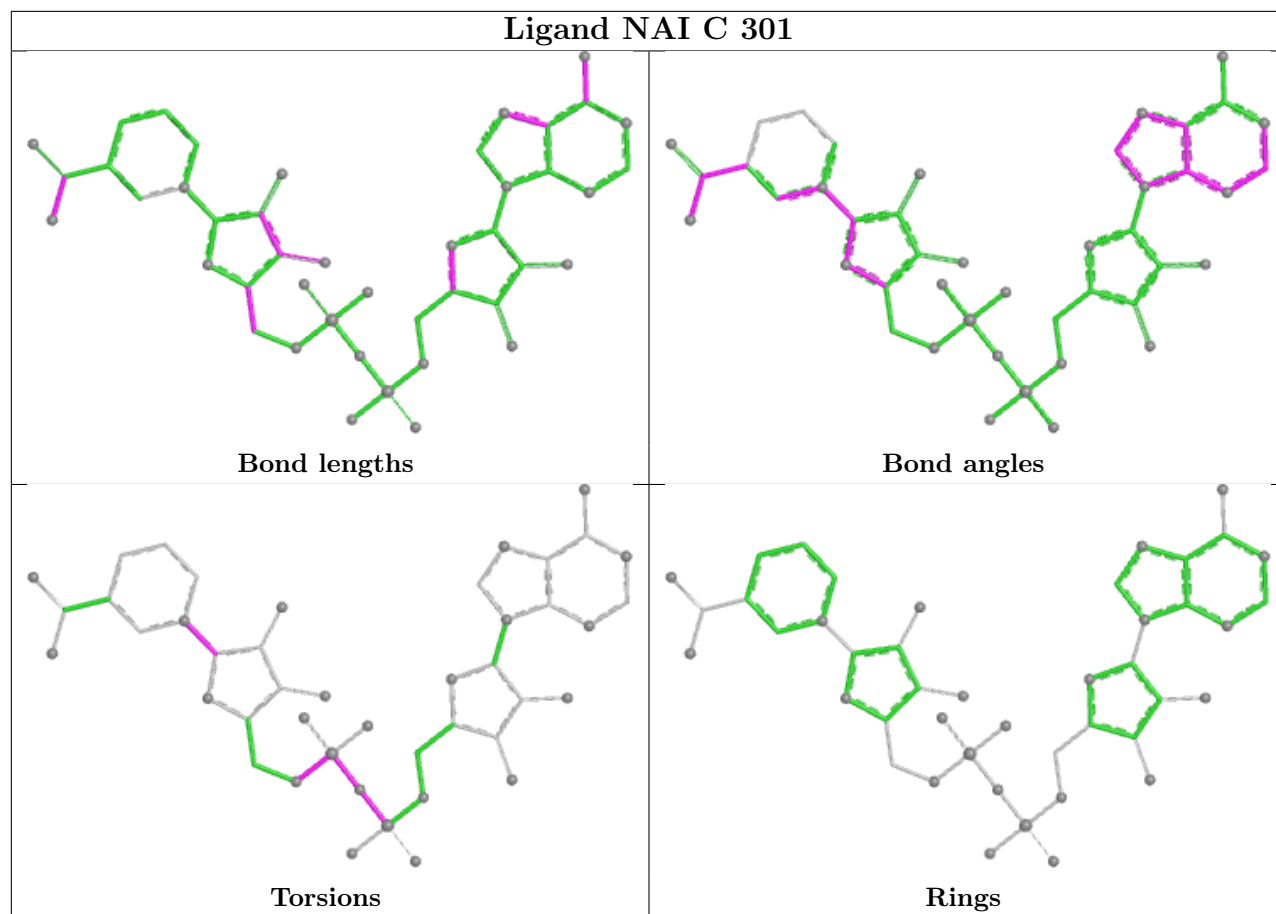
1 monomer is involved in 1 short contact:

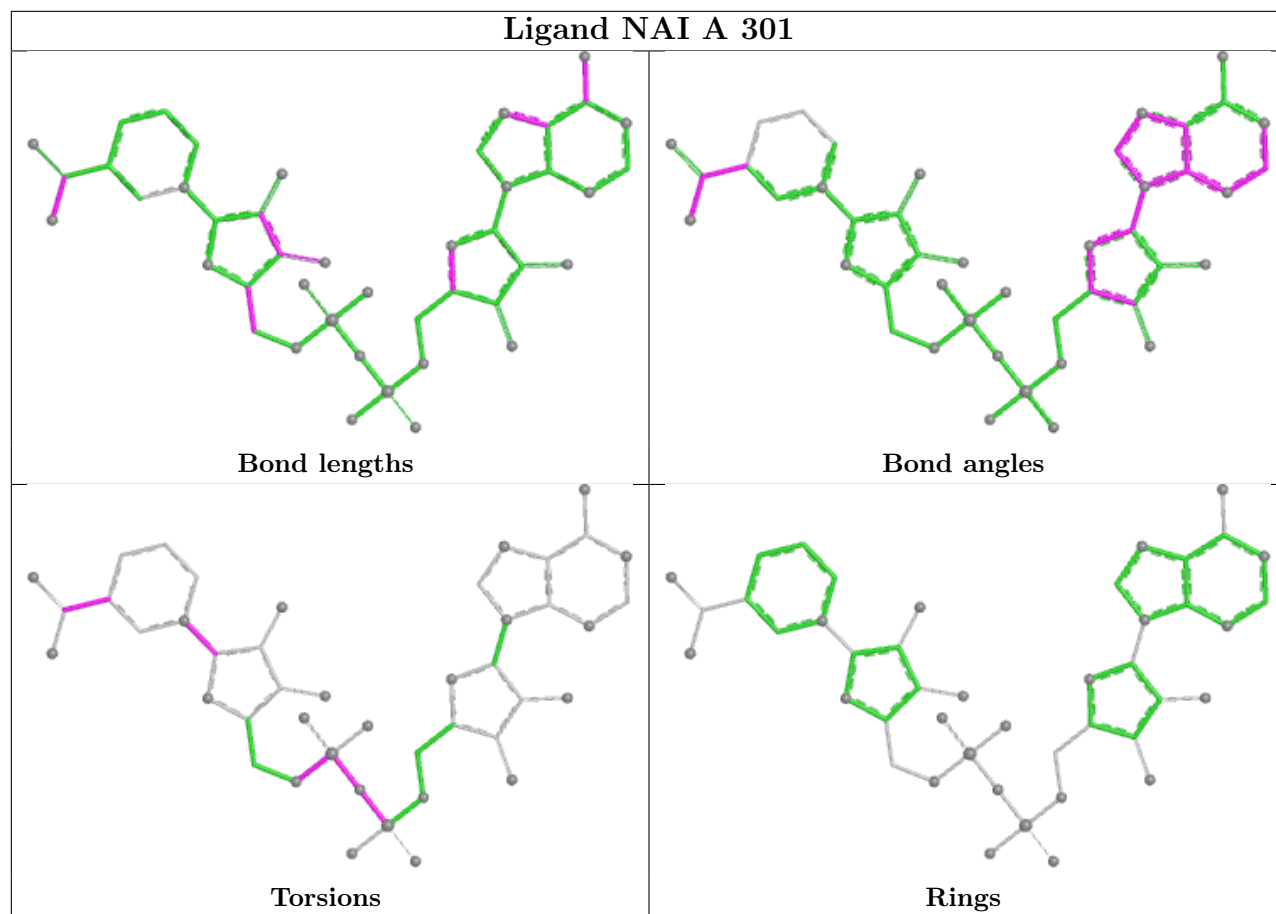
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	CAA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	242/250 (96%)	0.31	11 (4%) 38 49	8, 18, 37, 62	5 (2%)
1	B	244/250 (97%)	0.26	14 (5%) 29 40	8, 15, 37, 69	4 (1%)
1	C	242/250 (96%)	0.36	16 (6%) 24 34	8, 17, 39, 66	2 (0%)
1	D	242/250 (96%)	0.33	13 (5%) 31 42	10, 16, 40, 67	1 (0%)
All	All	970/1000 (97%)	0.31	54 (5%) 30 41	8, 16, 40, 69	12 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	VAL	7.5
1	B	199	VAL	5.9
1	D	199	VAL	5.5
1	C	203	VAL	5.4
1	B	200	PRO	5.1
1	C	199	VAL	5.0
1	A	199	VAL	4.7
1	B	204	ILE	4.6
1	D	197	ALA	4.3
1	D	196	VAL	4.3
1	B	201	GLU	4.2
1	D	200	PRO	4.2
1	C	196	VAL	4.1
1	C	197	ALA	4.0
1	C	200	PRO	4.0
1	B	202	LYS	4.0
1	D	204	ILE	4.0
1	A	196	VAL	3.8
1	C	202	LYS	3.7
1	C	204	ILE	3.7
1	D	203	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	197	ALA	3.5
1	C	201	GLU	3.5
1	A	200	PRO	3.4
1	A	198	GLU	3.2
1	B	205	GLU	3.2
1	D	195	MET	3.1
1	D	178	ARG	3.0
1	B	198	GLU	2.9
1	B	207	MET	2.9
1	B	197	ALA	2.8
1	C	45	PHE	2.8
1	B	178	ARG	2.8
1	C	207	MET	2.7
1	A	203	VAL	2.7
1	B	196	VAL	2.7
1	D	74	HIS	2.6
1	C	9	SER	2.6
1	A	204	ILE	2.6
1	B	7	HIS	2.4
1	A	9	SER	2.4
1	A	84	PHE	2.4
1	D	202	LYS	2.4
1	B	8	MET	2.3
1	D	193	THR	2.3
1	C	210	GLN	2.2
1	C	190	PHE	2.2
1	C	198	GLU	2.2
1	D	198	GLU	2.2
1	A	206	LYS	2.2
1	D	206	LYS	2.2
1	C	206	LYS	2.1
1	C	178	ARG	2.0
1	A	207	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

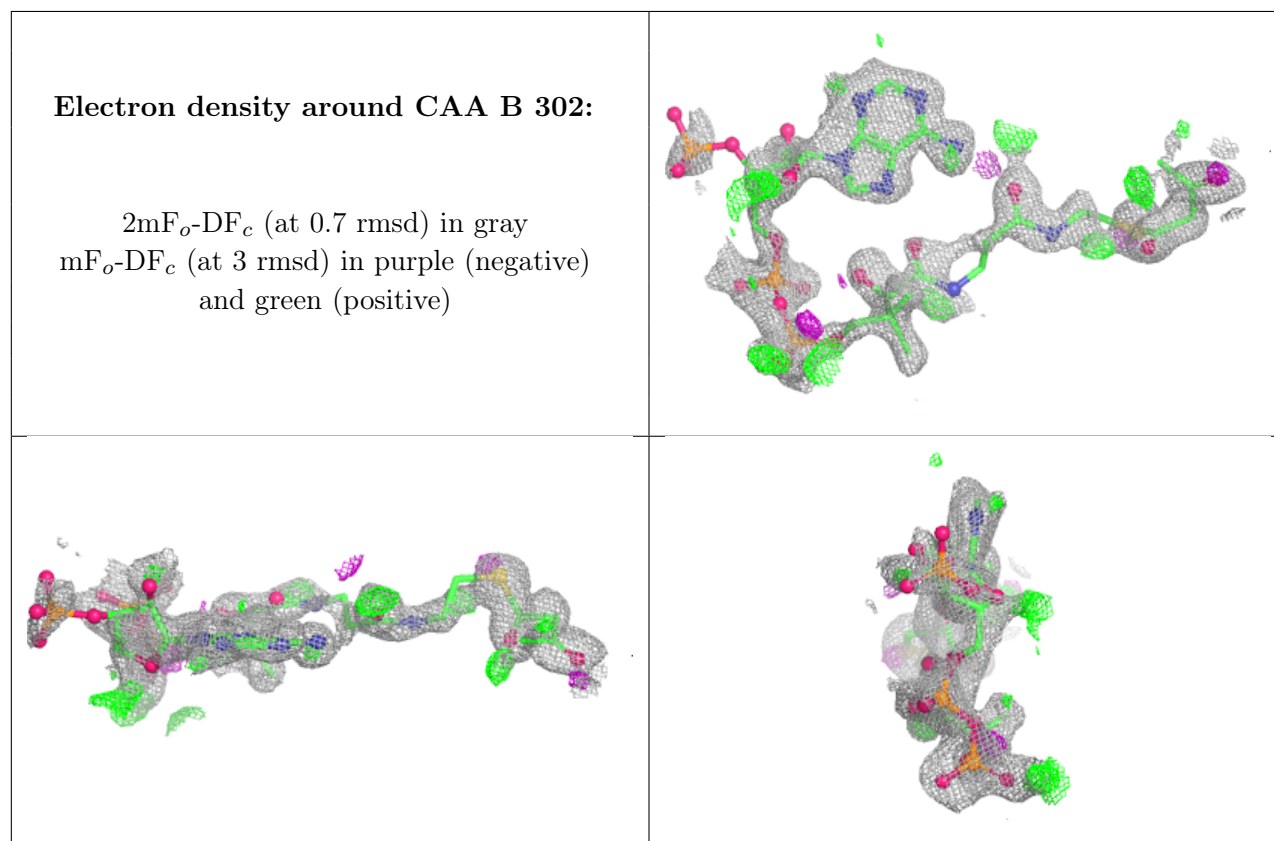
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

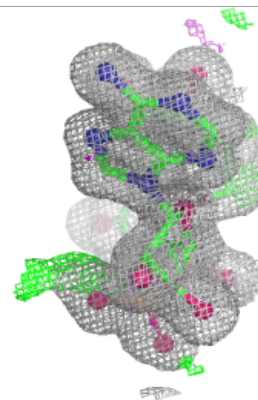
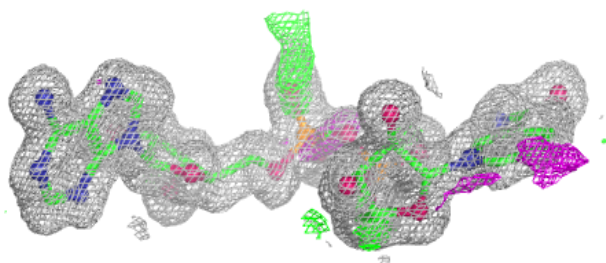
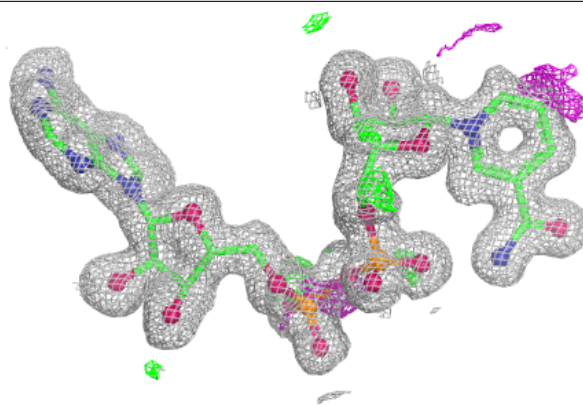
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CAA	B	302	54/54	0.79	0.17	19,42,97,98	54
2	NAI	B	301	44/44	0.97	0.06	10,13,16,21	0
2	NAI	C	301	44/44	0.97	0.06	11,14,18,23	0
2	NAI	D	301	44/44	0.97	0.06	11,14,19,27	0
2	NAI	A	301	44/44	0.97	0.06	11,14,18,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

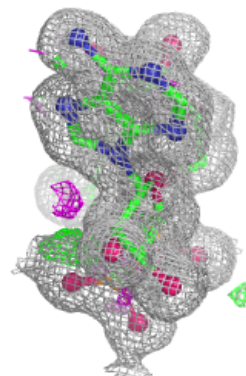
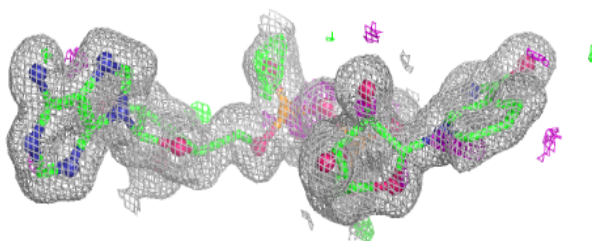
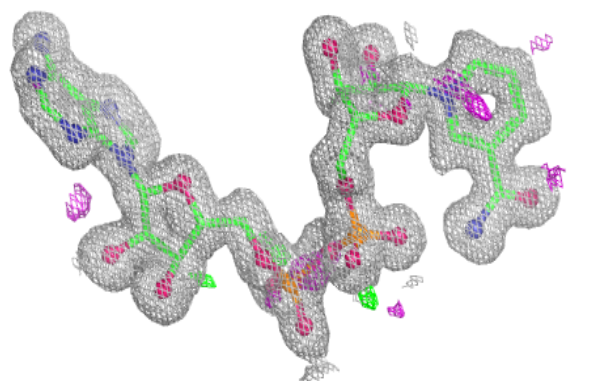


Electron density around NAI B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

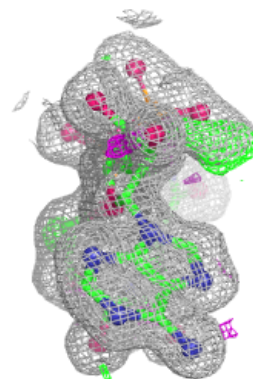
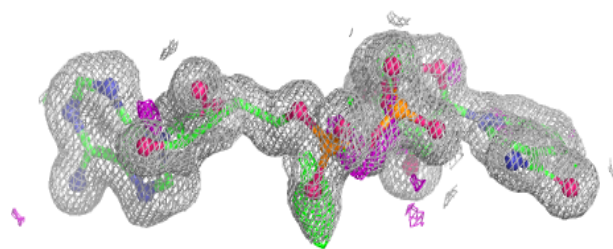
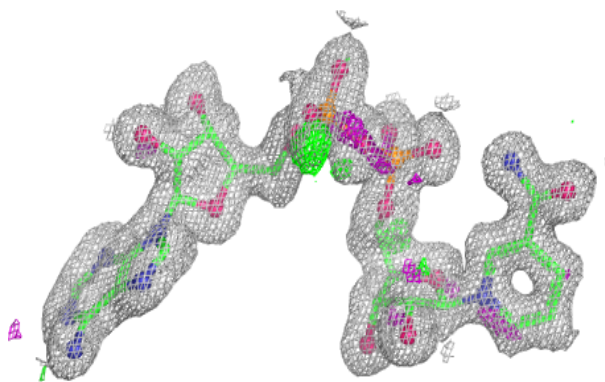
**Electron density around NAI C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

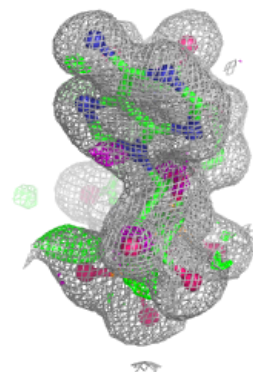
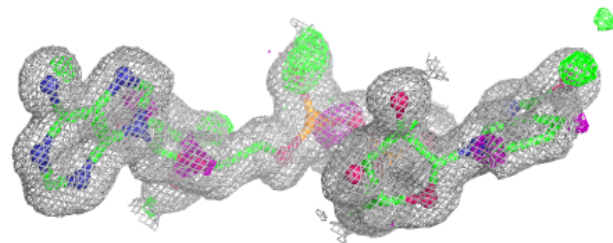
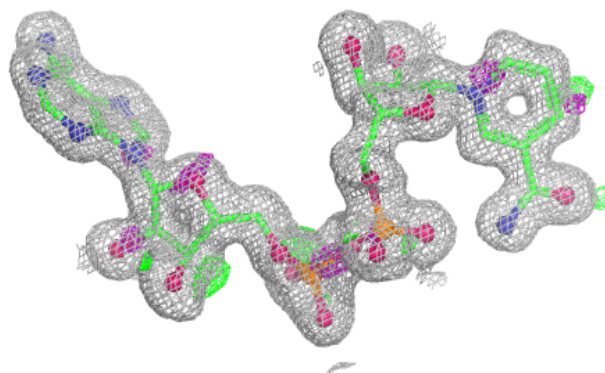


Electron density around NAI D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAI A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.